Sebacic acid, but-3-yn-2-yl hexyl ester

Inchi: InChI=1S/C20H34O4/c1-4-6-7-14-17-23-19(21)15-12-10-8-9-11-13-16-20(22)24-18(3)5-2
InchiKey: FAKWWYFKCHDNSD-UHFFFAOYSA-N
Formula: C20H34O4
SMILES: C#CC(C)OC(=O)CCCCCCCCC(=O)OCCCCCC
Mol. weight [g/mol]: 338.48

Physical Properties

Property code	Value	Unit	Source
gf	-129.69	kJ/mol	Joback Method
hf	-659.11	kJ/mol	Joback Method
hfus	52.58	kJ/mol	Joback Method
hvap	77.90	kJ/mol	Joback Method
log10ws	-5.83		Crippen Method
logp	4.796		Crippen Method
mcvol	298.940	ml/mol	McGowan Method
pc	1197.30	kPa	Joback Method
rinpol	2291.00		NIST Webbook
tb	799.26	K	Joback Method
tc	985.84	K	Joback Method
tf	491.45	K	Joback Method
vc	1.159	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	914.25	J/mol×K	799.26	Joback Method
cpg	931.55	J/mol×K	830.36	Joback Method
cpg	947.86	J/mol×K	861.45	Joback Method
cpg	963.20	J/mol×K	892.55	Joback Method
cpg	977.60	J/mol×K	923.65	Joback Method
cpg	991.06	J/mol×K	954.75	Joback Method
cpg	1003.62	J/mol×K	985.84	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355848&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume